

REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-05-

0074

The public reporting burden for this collection of information is estimated to average 1 hour per response, including gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments of information, including suggestions for reducing the burden, to Department of Defense, Washington Headquarters (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that any penalty for failing to comply with a collection of information if it does not display a currently valid OMB number.

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

ces.
ction
ports
all be

1. REPORT DATE (DD-MM-YYYY)			2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 15 Jul 2002 - 30 Sep 2004	
4. TITLE AND SUBTITLE Dynamic Structure LES Models					5a. CONTRACT NUMBER	
					5b. GRANT NUMBER F49620-02-1-0348	
					5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Christopher J. Rutland					5d. PROJECT NUMBER	
					5e. TASK NUMBER	
					5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Engine Research Center Department of Mechanical Engineering University of Wisconsin - Madison Madison WI 53706					8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) USAF/AFRL AFOSR 801 N. Randolph Street Arlington VA 22203 NA					10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR	
					11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Distribution Statement A. Approved for public release; distribution is unlimited.						
13. SUPPLEMENTARY NOTES						
14. ABSTRACT A new dynamic structure (DS) approach for large eddy simulation modeling has been developed. The approach uses a tensor coefficient for the structure of the sub-grid stresses and a sub-grid kinetic energy for the magnitude of the stresses. The tensor coefficient is obtained directly from using the common "'dynamic approach' using the Germano identity. The sub-grid kinetic energy is obtained from a transport equation. The objectives of the program are: (i) to develop the DS approach for scalar transport with potential application to heat transfer problems and (ii) develop and test the DS formulation for rotating turbulence. The approach offers several significant advantages over existing approaches including: (i) no turbulent viscosity is used, (ii) an energy budget is enforced, (iii) very good prediction of the actual sub-grid stresses is obtained, and (iv) the model rests on a sound mathematical foundation that observes solvability constraints. New subgrid scale models are developed for subgrid scalar flux, subgrid scalar dissipation and subgrid scale energy dissipation. Models are evaluated a-priori using available DNS data for decaying isotropic turbulence, incompressible channel and Couette flows, and non-reacting mixing layer. A posteriori tests include LES of decaying isotropic turbulence and LES of incompressible mixing layer.						
15. SUBJECT TERMS						
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 14	19a. NAME OF RESPONSIBLE PERSON	
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U			19b. TELEPHONE NUMBER (Include area code)	

FINAL REPORT

DYNAMIC STRUCTURE LES MODELS

AFOSR GRANT NUMBER: F49620-02-1-0348

Christopher J. Rutland
Engine Research Center
Department of Mechanical Engineering
University of Wisconsin - Madison

Abstract

A new dynamic structure (DS) approach for large eddy simulation modeling has been developed. The approach uses a tensor coefficient for the structure of the sub-grid stresses and a sub-grid kinetic energy for the magnitude of the stresses. The tensor coefficient is obtained directly from using the common 'dynamic approach' using the Germano identity. The sub-grid kinetic energy is obtained from a transport equation. The objectives of the program are: (i) to develop the DS approach for scalar transport with potential application to heat transfer problems and (ii) develop and test the DS formulation for rotating turbulence. The approach offers several significant advantages over existing approaches including: (i) no turbulent viscosity is used, (ii) an energy budget is enforced, (iii) very good prediction of the actual sub-grid stresses is obtained, and (iv) the model rests on a sound mathematical foundation that observes solvability constraints. New subgrid scale models are developed for subgrid scalar flux, subgrid scalar dissipation and subgrid scale energy dissipation. Models are evaluated *a-priori* using available DNS data for decaying isotropic turbulence, incompressible channel and Couette flows, and non-reacting mixing layer. *A posteriori* tests include LES of decaying isotropic turbulence and LES of incompressible mixing layer.

Background

The next generation of turbulent flow simulations will undoubtedly use large eddy simulation (LES) modeling approaches (Moin 1997, Ferziger 1983). However, the adoption of LES for more general use has been slow, in large part due to the very large, nearly DNS, grids that are required. One could attribute the large grid size requirements to limitations of the current modeling approaches. Recently, a new approach, called dynamic structure modeling (Pomraning 2000, Pomraning and Rutland 2002), has been developed that offers several important advantages over existing LES approaches.

In LES, spatial filtering is used to remove scales that must be resolved in the simulation. When applied to incompressible, non-reacting turbulent flow, the basic term that requires modeling for is the sub-grid stress tensor:

$$\tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \quad (1)$$

where the over-bar indicates LES spatial filtering. The dynamic Smagorinsky approach is the most commonly used for current applications. This model assumes that the stress tensor, τ_{ij} , can be linearly related to the resolved scale strain rate tensor:

$$\tau_{ij} \approx -\nu_T \overline{S_{ij}} \quad (2)$$

where $\overline{S_{ij}}$ is the resolved scale strain rate tensor and ν_T is a 'turbulent' viscosity commonly modeled as $\nu_T = C_s \Delta^2 |\overline{S}|$ with Δ a representative length scale and C_s a modeling coefficient. (Note, for clarity a trace term, commonly absorbed into the incompressible pressure, is not shown.) This is a turbulent viscosity based model, and any model based on a viscosity approach will require a positive viscosity coefficient for numerical stability. This means that the sub-grid model is only a dissipative term and removes kinetic energy from the flow. However, τ_{ij} is not a purely dissipative term – it is a local term, because LES filtering is a local operation. Moreover, the application of eddy viscosity models in LES violates one of the basic assumptions of gradient modeling – that the length scale of the modeled phenomena is significantly smaller than the distance over which the mean gradient changes appreciably, as pointed out by Corrsin (Corrsin 1974).

The dynamic approach uses another 'test' level filtering operation (indicated by a peaked over-bar) and a new tensor arising from the Germano identity (Germano 1991):

$$L_{ij} = \overline{\widehat{u_i u_j}} - \widehat{\overline{u_i u_j}} \quad (3)$$

This tensor is known from the resolved scale and can be used to formulate the following equation for the model coefficient in the dynamic Smagorinsky model:

$$L_{ij} - \frac{1}{3} \delta_{ij} L_{kk} = \alpha_{ij} C_s - \beta_{ij} \widehat{C_s} \quad (4)$$

where $\alpha_{ij} = -2\widehat{\Delta}^2 |\widehat{S}| \widehat{S_{ij}}$ and $\beta_{ij} = -2\Delta^2 |\overline{S}| \overline{S_{ij}}$ are introduced for notational simplicity. This is an extra equation that can be used to solve for either the viscosity directly or the model coefficient in the viscosity of Eq. (2). However, Eq. (4) is a second rank tensor equation (e.g. six equations by symmetry) for a single unknown coefficient, C_s . This highly over specified situation is commonly dealt with by using a minimization procedure to find the coefficient. We note that this over specification could be interpreted as a fairly fundamental problem with the whole dynamic Smagorinsky approach.

There are two other approaches in LES modeling due to Ghosal et al. (1995) and Menon et al. (1995). Both of these use a sub-grid kinetic energy and this represents an advance over the zero equation Smagorinsky approach. However, both approaches use the kinetic energy only as an additional scaling term to form a turbulent viscosity. Thus, they still follow Eq. (2) and suffer from the same inherent limitations.

The Dynamic Structure Approach

To address some of the mathematical and conceptual difficulties in the common LES models, a new modeling approach was developed. This new approach does not use a turbulent viscosity concept, but instead attempts to model the sub-grid stresses directly. This is accomplished by using the following model where k is the subgrid kinetic energy:

$$\tau_{ij} = c_{ij} k \quad k = \frac{1}{2} (\overline{u_i u_i} - \overline{u_i} \overline{u_i}) \quad (5)$$

and c_{ij} is a tensor coefficient that is obtained directly as part of the solution using the dynamic procedure. This is accomplished by defining a ‘test’ level model:

$$T_{ij} = c_{ij} K \quad K = \frac{1}{2} \left(\widehat{u_i u_i} - \widehat{u_i} \widehat{u_i} \right) = \hat{k} + \frac{1}{2} L_{ii} \quad (6)$$

using the test level kinetic energy, K , can be written as a function of the sub-grid kinetic energy and the trace of the L_{ij} tensor. Then the Germano identity is used to formulate an equation for the tensor coefficient, c_{ij} :

$$L_{ij} = K c_{ij} - \widehat{k c_{ij}} \quad (7)$$

Note that this is a well-posed problem in that the number of coefficient unknowns matches the number of equations. Fundamentally this is an integral equation for the coefficient tensor (e.g. the over-bar indicates an integral filter) and we have tested it in the integral form (Pomraning 2002). However, a very effective algebraic form of the model is formulated by assuming that the coefficient tensor can be brought outside the integral. Then, the dynamic structure model becomes:

$$\tau_{ij} = (L_{ij} / L_{kk}) 2k \quad (8)$$

Here the sub-grid kinetic energy is obtained from a transport equation. Thus, the dynamic structure model is a one-equation, non-turbulent viscosity model. The tensor structure of the sub-grid stress tensor, τ_{ij} , is found directly from the dynamic approach through the tensor coefficient. This is very advantageous because the coefficient is just the normalized L_{ij} tensor, which is directly related to the structure of the sub-grid stresses (see Eq. (3)).¹ Then, the magnitude of τ_{ij} is obtained from the sub-grid kinetic energy, k , which is simply twice the trace of τ_{ij} itself.

Advantages of the New Approach

1. Non-viscosity based – By not using a turbulent viscosity approach, the dynamic structure model is not purely dissipative. This allows local solutions that respond to the local flow conditions – conditions that are not always dissipative. This suggests that the model has the potential to give the correct behavior in flows with streamline curvature or system rotation that often cause traditional approaches difficulty. There is no turbulent viscosity in the new model and molecular viscosity plays its correct physical role of dissipating sub-grid energy.
2. An energy budget – The dynamic structure model has a sub-grid transport equation for k . Hence it is a one-equation model rather than a zero equation model like the dynamic Smagorinsky model. This energy budget keeps the model stable without a turbulent viscosity. Hence, it is very robust and works over a wide range of grid resolutions including practical situations in which there is significant energy in the sub-grid scales.

¹ Note that Meneveau group (Meneveau and Katz 2000, Liu et al. 1998) once suggested a similar idea but did not find the appropriate scaling for the magnitude of the sub-grid stress tensor.

Dynamic Smagorinsky models require dense grids with little energy in the sub-grid scales so that the sub-grid model is not required to do much.

3. Good prediction of the sub-grid stresses – The component structure, spatial distribution, and magnitude of the sub-grid stresses, τ_{ij} , are very well predicted by the new model. This is shown in Fig. 1 that compares the new model to the standard dynamic Smagorinsky model. Clearly the new model does a much better job of predicting the actual sub-grid stresses. This is due to the tensor coefficient that comes directly from using the stress tensor structure in the dynamic approach. This makes the new model a very strong candidate for flows with more complex physics such as heat transfer because the sub-grid terms can be used to build other sub-models.
4. Solvability – The mathematical formulation of the new model is much sounder than the common dynamic Smagorinsky model. The underlying formulation of the dynamic approach is a Fredholm integral equation of the second kind that has specific solvability constraints. Other LES formulations that relate τ_{ij} to \bar{S}_{ij} can be shown to violate solvability criteria for almost any type of flow. However, the dynamics structure model relates τ_{ij} to the sub-grid kinetic energy and this results in integral equations that easily satisfy solvability. This sound mathematical formulation adds robustness to the model so that it works under a wide variety of flows and grid resolutions. Additionally, it also appears to guarantee other nice properties such as realizability (e.g. non-negative diagonal stress components). Finally, we note that the model is Galilean invariant (Pomraning 2002).

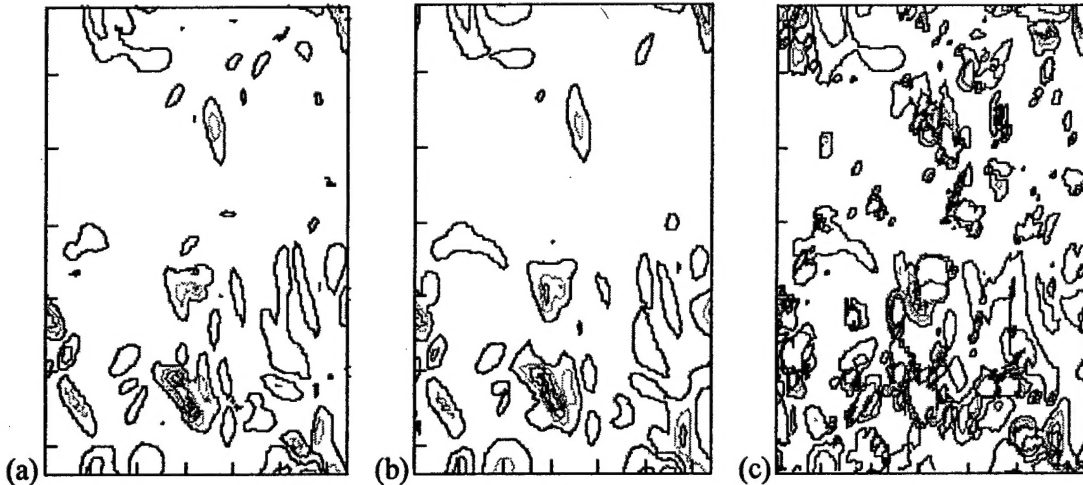


Figure 1: Results from isotropic decaying turbulence; contours of the τ_{12} sub-grid shear stress: (a) DNS result, (b) dynamic structure model, (c) dynamic Smagorinsky model

The dynamic structure model (Eq. (8)) has been tested in a high order LES code for isotropic turbulence and compared very well with Comte-Bellot results (Pomraning 2002). Note, unlike many Smagorinsky based models, the sub-grid kinetic energy accounted for a significant portion of the total kinetic energy, often 10% or more.

The model has also been applied to other problems in a low-order ‘engineering’ code. While there are issues of numerical accuracy in these codes, this is somewhat mitigated by the higher Reynolds numbers and coarser grid resolutions that require larger magnitudes of the model terms. Some results are shown for the Eaton *et al.* (1986) backwards-facing

step in Figure 2. These results required time averaging of the LES results to achieve the appropriate comparison with the time averaged experimental results. This figure also shows the results of using no model to demonstrate that the numerical dissipation is not providing the correct sub-grid model.

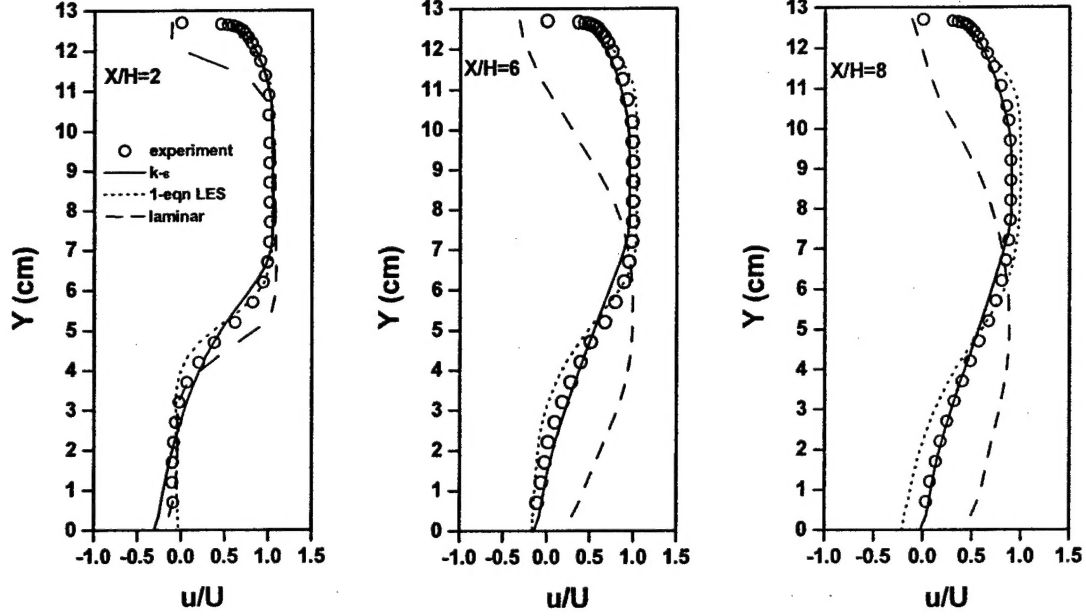


Figure 2: Normalized streamwise velocity profiles at three locations downstream of a backwards facing step; comparisons between experimental data of Eaton *et al.* [9], a $k-\epsilon$ case, the dynamic structure model, and a no-model (e.g. 'laminar') case.

LES Equations for Scalar Transport

The LES transport equation for a scalar ϕ is obtained by applying the spatial filtering operation to the original transport equation to yield:

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial \bar{u}_j \bar{\phi}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[D \frac{\partial \bar{\phi}}{\partial x_j} \right] - \frac{\partial \tau_{j,\phi}}{\partial x_j}. \quad (9)$$

Here, $\bar{\phi}$ denotes the spatially averaged scalar ϕ , D is the diffusion coefficient, and $\tau_{j,\phi} = \bar{u_j \phi} - \bar{u_j} \bar{\phi}$ is the subgrid-scale (SGS) flux term which has to be modeled. The most popular models are gradient-type models:

$$\tau_{j,\phi} \approx \mu_T \frac{\partial \bar{\phi}}{\partial x_j} = C_s \Delta^2 |S_{kl}| \frac{\partial \bar{\phi}}{\partial x_j}. \quad (10)$$

Various techniques for determination of the turbulent viscosity μ_T have been proposed (Kim *et al.* 1999; Kimmel and Domaradzki 2000). The dynamic viscosity approach uses another filtering operation referred to as "test" filtering and denoted by $\hat{\phi}$ (Germano *et al.* 1991). Similar to models for SGS Reynolds stress, the eddy viscosity models are hardly applicable for turbulence modeling, as outlined by Corrsin (1974). Another approach is to use self-similarity models of the type

$$\tau_{j,\phi} \approx C \left[\widehat{u_j \phi} - \widehat{u_j} \widehat{\phi} \right], \quad (11)$$

where C is a scaling constant, or mixed models that combine (10) and (11) (Speziale et.al. (1988))

Dynamic Structure Models for SGS Scalar Flux and Scalar Dissipation

In the spirit of the model (8) developed by Pomraning and Rutland (2002), we propose the following model for the subgrid scalar flux:

$$\tau_{i,\phi} \approx \frac{\theta}{\Theta} L_{i,\phi} \equiv \frac{\overline{\phi\phi} - \widehat{\phi}\widehat{\phi}}{\widehat{\phi}\widehat{\phi} - \widehat{\phi}\widehat{\phi}} \left[\widehat{u_i\phi} - \widehat{u_i}\widehat{\phi} \right]. \quad (12)$$

Here $\theta = \overline{\phi\phi} - \widehat{\phi}\widehat{\phi}$ is the SGS variance of ϕ on the base (grid) level, $\Theta = \widehat{\phi}\widehat{\phi} - \widehat{\phi}\widehat{\phi}$ is the SGS variance of ϕ on the test level, and $L_{i,\phi} = \widehat{u_i\phi} - \widehat{u_i}\widehat{\phi}$ is the modified Leonard-type term for scalar equation. Note that the SGS variance θ cannot be obtained from the resolved quantities and thus has to be modeled (Cook and Riley, 1994; Pierce and Moin; 1998) or obtained from a separate transport equation (Jimenez et.al, 2001). In keeping with the DS approach, we use a transport equation for θ that can be obtained from (9):

$$\frac{\partial \theta}{\partial t} + \frac{\partial \overline{u_j\theta}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[D \frac{\partial \theta}{\partial x_j} \right] - \chi_\theta - C_\theta + \phi \frac{\partial \tau_{j,\phi}}{\partial x_j}, \quad (13)$$

where

$$\chi_\theta = 2D \left[\frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} - \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \right] \quad \text{and} \quad C_\theta = \frac{\partial}{\partial x_j} \left[\overline{\phi^2 u_j} - \widehat{\phi^2 u_j} \right]$$

are the SGS scalar dissipation term and triple correlation term, respectively. The triple correlation term is usually either omitted or modeled using gradient-type models. Alternatively, it is possible to approximate the sum of last two terms in the transport equation for θ to the third order of computational mesh spacing using the series given by Bedford and Yeo (1993). The resulting equation is:

$$\frac{\partial \theta}{\partial t} + \frac{\partial \overline{u_j\theta}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[D \frac{\partial \theta}{\partial x_j} \right] - \chi_\theta - \tau_{j,\phi} \frac{\partial \phi}{\partial x_j} \quad (14)$$

where the subgrid flux is modeled using (12) and the SGS scalar dissipation is modeled using its own modified Leonard type term:

$$\chi_\theta \approx 2 \frac{\theta}{\Theta} L_\chi \equiv 2 \frac{\theta}{\Theta} \left[\frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} - \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \right] \quad (13)$$

A priori Test

The scalar flux and scalar dissipation models were tested using a DNS data for non-reacting incompressible spatially developing mixing layer from Mason and Rutland (2000). The Reynolds number based on the inlet vorticity thickness was 200. For the purpose of the *a priori* testing, the modeled quantities were computed directly from the DNS data using filtered DNS results and the LES models. In order to test robustness of the models, LES filters of various dimensions were applied to the DNS data. The DS

models for the SGS scalar flux and SGS scalar dissipation were compared to several models in the literature.

Figure 3a represents the results of comparison of the DS model (12) and a viscosity gradient model (10). The DS model has a smaller data scatter indicating that it performs better. These comparisons were made over a range of LES filter sizes and shapes and the DS model performed better in all cases (Chumakov and Rutland, 2003)

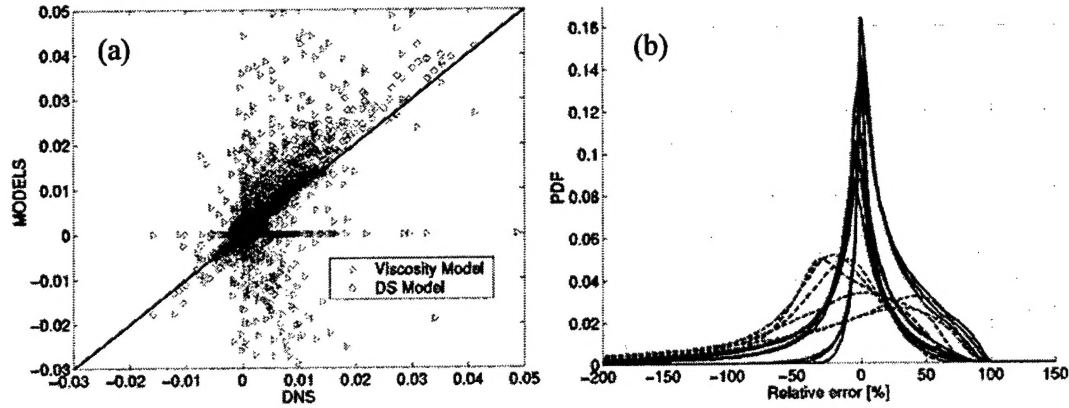


Figure 3: (a) Scatter plot of SGS scalar flux term computed from DNS and using DS model (blue circles) and viscosity models (red triangles) (b) PDF of relative error for models of the SGS dissipation term: DS model (blue solid) and Jimenez et al. (2001) (red dashed). Different curves represent different LES filters shapes and sizes.

Figure 3b depicts the results of a similar *a priori* test for two SGS dissipation models. The DS model (12) is compared to the one from Jimenez et.al (2001)

$$\chi_0 = \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \approx C_0 \frac{\varepsilon_0}{k} \theta,$$

where $\varepsilon_0 = \overline{\nu(\partial u_i / \partial x_j \partial u_i / \partial x_j)}$ is the SGS kinetic energy dissipation. Note that this model is similar to a RANS type models in that it uses a turbulence time scale for the scalar dissipation. Experience has shown that this time scale is often not appropriate for scalar quantities, for example in turbulent regions where the scalar quantity has become uniform from mixing. Figure 1b shows a PDF plot of the *a priori* error for the scalar dissipation models. The DS model performs better with errors centered at zero and smaller spread.

Subgrid Scale Energy Dissipation

The SGS kinetic energy is obtained from a transport equation, which requires a model for SGS energy dissipation

$$\varepsilon_{SGS} = \nu \left[\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right].$$

Together with the energy transfer term $\Pi = \tau_{ij} S_{ij}$, the SGS dissipation plays a crucial role in the energy transfer process between the turbulence scales. While Π is responsible for the energy transfer between the resolved and unresolved scales, ε removes the energy from the unresolved scales. A model has been tested for ε which has the

form $\varepsilon_{SGS} \approx \nu \cdot F \cdot L_\varepsilon$ where L_ε is the Leonard type term associated with dissipation (see Eq. (14)). The scaling factor F was investigated from *a priori* tests. Three DNS datasets of decaying isotropic with $Re_\lambda \approx 104.5, 92.6$, and 53.7 were used. The proposed form of the scaling factor F is: $F = C_\varepsilon [k/K]^\gamma$, where $2K = L_{ii} = \widehat{u_i u_i} - \widehat{u_i} \widehat{u_i}$ is the trace of the Leonard term, and C_ε and γ are the constants to be determined from the *a priori* study. Probability density functions (PDFs) for C_ε show a good collapse for $\gamma = 1/2$. An additional dependence on the base filter to the $3/2$ power was also seen. Thus, a length scale ratio was added to F so that the form of the model is:

$$\varepsilon_{SGS} \approx \nu \cdot C \left[\frac{\Delta}{l} \right]^{3/2} \sqrt{\frac{k}{K} \left[\frac{\widehat{\partial u_i \partial u_i}}{\partial x_j \partial x_j} - \widehat{\partial u_i} \widehat{\partial u_i} \right]} \quad (14)$$

where, C is a scaling constant and l is a base filter level length scale, both to be determined in future work.

Limiting Behavior of Dynamic Structure Models

Dynamic structure models use ratio of variances as a scaling factor. We examine the limiting behavior of the scaling factors θ/Θ and $2k/L_{mm}$ for the case when the denominator of the scaling factor goes to zero. This can occur when either the grid is asymptotically refined ($\Delta \rightarrow 0$), or the flow field becomes quiescent, for example in the far-field of a jet. For simplicity, only θ/Θ is presented. Using a Leonard expansion (Bedford and Yeo (1993), Leonard (1974)) one can show that for both cases the scaling factor stays bounded by minimum and maximum of ratios of directional second moments of the base and test filters, i.e.,

$$0 < \min \frac{\alpha}{\hat{\alpha}} \leq \frac{\theta}{\Theta} \leq \max \frac{\alpha}{\hat{\alpha}} < \infty, \text{ where } \alpha_i = \int_{-\infty}^{\infty} x_i^2 G(x) dx_i, \quad \hat{\alpha}_i = \int_{-\infty}^{\infty} x_i^2 \hat{G}(x) dx_i.$$

This statement is illustrated for a one-dimensional scalar function ϕ . Figure 4 presents a scatter plot of the mean base variance θ vs. the mean scaling factor θ/Θ together with the line $y = \alpha/\hat{\alpha}$. The plot was obtained by successively filtering a random signal to obtain increasing smoother signals (and hence smaller variances). This shows that the mean value of the scaling factor goes to the ratio of $\alpha/\hat{\alpha}$ as the scalar field becomes quiescent as indicated by the diminishing SGS variance.

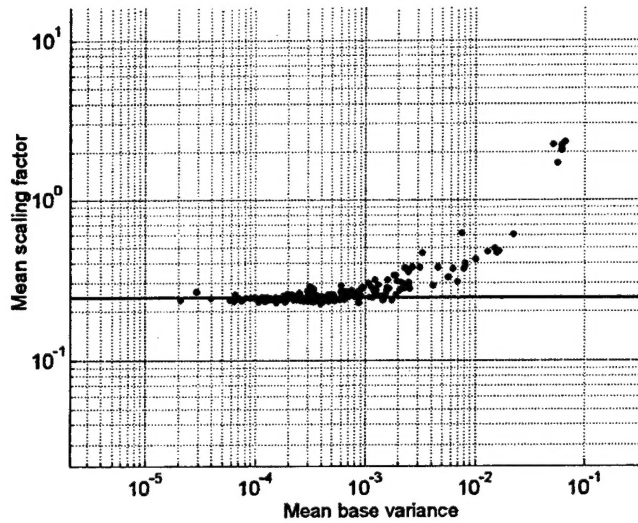


Figure 4. Scatter plot of the mean base SGS variance vs. the mean scaling factor, θ/Θ . The line represents the ratio $\alpha/\hat{\alpha}$ and indicates the limiting behavior.

A-posteriori Test – non-reacting incompressible mixing layer

In order to evaluate both DS models an LES simulation of a non-reacting incompressible spatially developing mixing layer was performed. All parameters in the LES simulation were as close to DNS parameters as possible but the LES used $1/4$ as many grid points in each coordinate direction. The first- and second-order statistics were computed at various locations downstream and then compared.

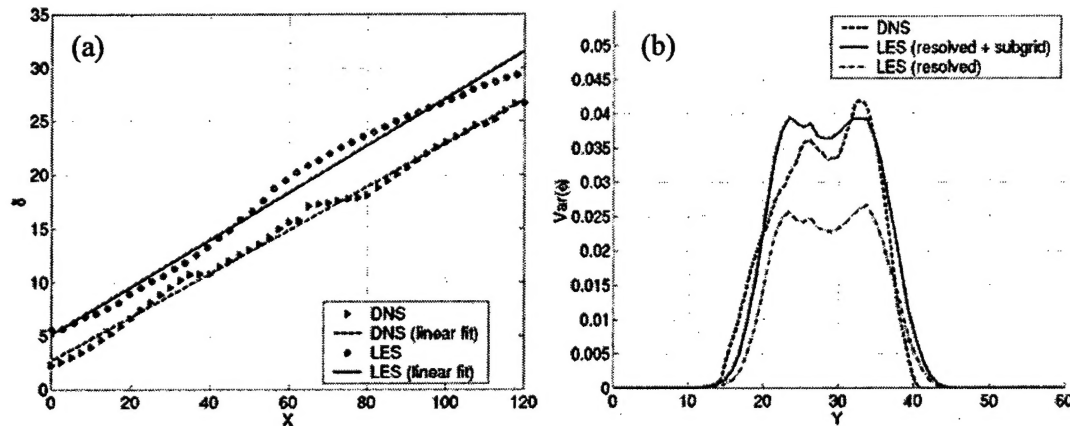


Figure 5: (a) Rates of growth for mixing layer based on 1% scalar difference: DNS and LES; (b) Comparison of the scalar variance for DNS and LES.

Figure 5a shows the comparison of first-order statistics from the DNS and LES runs. Both DNS and LES mixing layer exhibit linear rate of growth in the domain, as generally found in literature (Dimotakis, 1991). The growth rate was determined using the 1% passive scalar thickness and a velocity ratio of $1/3$. The growth rate coefficient for the LES was found to be 0.455. This is similar to the DNS value of 0.422 and close to the experimentally accepted range of 0.25 to 0.45. Figure 4b shows the comparison between the LES and DNS mean scalar profiles near the end of the computational domain.

The variance of the passive scalar from the DNS and LES simulations is presented in Figure 5b. There is good agreement in magnitude and spanwise distribution. Note that there is a large contribution from the subgrid variance θ to the total variance of the scalar – a characteristic common of DS type models.

A-posteriori Test – decaying isotropic turbulence

LES of decaying isotropic turbulence is a good test for both the SGS stress, τ_{ij} , model and the SGS energy dissipation, ε_{SGS} , model. In general, decaying turbulence exhibits two different types of behavior: an inertia-dominated earlier stage, and viscosity-dominated (final) stage (Pope 2000). The energy decay rate for the final period can be obtained analytically from the Karman-Howarth equation, which yields $E \sim t^{-5/2}$. For the inertia-dominated period, only experimental measurements are known, but the total kinetic energy clearly exhibits the power-law decay suggested by Comte-Bellot and Corrsin (1966): $E \sim t^{-n}$. The values of the decay exponent n between 1.15 and 1.45 are reported in the literature but Mohammed and LaRue (1990) suggested that nearly all of the data are consistent with $n=1.3$. Thus we match the energy decay rate given by LES against the power law with $n=1.3$ for the inertia-dominated period, and $n=2.5$ for the final period.

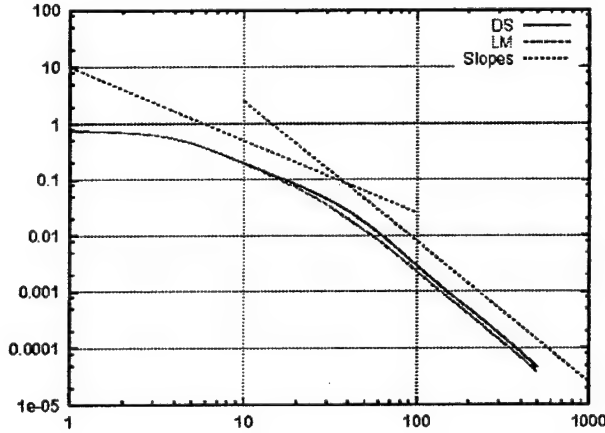


Figure 6. Decay of total kinetic energy in time. Slopes for $n=1.3$ and $n=2.5$ are plotted. (Initial Taylor scale Reynolds number = 200, grid size 32^3 .)

The dynamic structure model and another k -equation LES model are compared. The other model is a viscosity based model and uses $\tau_{ij} \approx -0.05\sqrt{k}\Delta S_{ij}$, $\varepsilon \approx 1.0k^{3/2}/\Delta$ ("Localization models", LM, Ghosal et al. 1995, Kim and Menon 1995, Menon et. al, 1996). Figure 6 shows the log-log plot of the decay of total kinetic energy in time for both models, along with the slopes for $n=1.3$ and $n=2.5$. In the LM run, the transition to the final phase of the flow is more spread out in time – approximately between $t=20\dots60$, as opposed to between $t=30\dots50$ for the DS run. The main difference between the two models is the ratio of energy in the subgrid scales to the total kinetic energy. In the latter stages of decay this ratio should diminish. This was seen only in the DS model. The LM model showed a nearly constant ratio of ~ 0.1 throughout the simulation (Chumakov and Rutland 2005).

Rotating Flows

The dynamic structure approach is being extended to simulate rotating flows. Since the DS approach maintains an energy budget between resolved and subgrid scales, it is a good

candidate for modeling rotating flows in which there can be strong energy transfer to larger scales. The subgrid k equation in the DS approach does not require modification since the Coriolis term only appears in the momentum equation. Thus, efforts are focused on studying the subgrid stresses in rotating systems.

In a rotating frame of reference, the subgrid stresses are modified. Models for the subgrid stresses should also be modified to maintain a material frame indifference, MFI, (see Speziale, 1985, and Shimomura, 1999). Two models which observe MFI are:

$$\tau_{ij} = \left(\frac{\Upsilon_{ij}}{\Upsilon_{mm}} \right) 2k_{sgs} \quad \text{and} \quad \tau_{ij} = \left(\frac{G_{ij}}{G_{mm}} \right) 2k_{sgs} \quad (15)$$

$$\text{where:} \quad \Upsilon_{ij} = \overline{u_i u_j} - \hat{u}_i \hat{u}_j + C_c \left[\left(\overline{u_i u_j} - \hat{u}_i \hat{u}_j \right) + \left(\overline{u_i u_j} - \hat{u}_i \hat{u}_j \right) - 2 \left(\overline{u_i u_j} - \hat{u}_i \hat{u}_j \right) \right] \quad (16)$$

$$G_{ij} = \frac{\partial \bar{u}_i}{\partial x_k} \frac{\partial \bar{u}_j}{\partial x_k} \quad (17)$$

Both of these models use the dynamic structure methodology of using a subgrid kinetic energy to scale a normalized tensor. In equation (16) the first terms on the right-hand-side are the modified Leonard terms that appear in the original DS model. The additional terms in brackets represent a cross correlation term is required to maintain MFI. The cross correlation terms are modeled using an additional filtering level and a coefficient, C_c , of $O(1)$ (set to 1.5 below). In the second model (17), the nonlinear term G_{ij} is derived by Taylor expansion. It is tested because it maintains MFI.

Two correlation coefficients, defined in Figure 7, are used for *a priori* testing: The first, ρ_1 , is the correlation coefficient (e.g. the scatter), and the second, ρ_2 , is the regression coefficient (e.g. the slope of the scatter line). Each correlation goes to unity when a and b are perfectly correlated.

$$\rho_1 = \frac{\langle ab \rangle - \langle a \rangle \langle b \rangle}{\sqrt{(\langle a^2 \rangle - \langle a \rangle^2)(\langle b^2 \rangle - \langle b \rangle^2)}}$$

$$\rho_2 = \frac{\langle ab \rangle - \langle a \rangle \langle b \rangle}{\langle a^2 \rangle - \langle a \rangle^2}$$

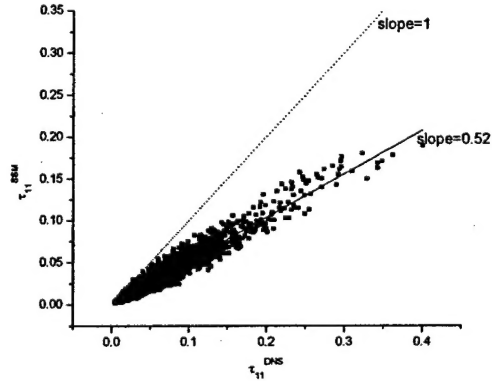


Figure 7: Definition of correlation coefficients and an example scatter plot. In this example case for a scale-similarity model $\rho_1 = 0.960$ and $\rho_2 = 0.519$.

Results of two *a priori* tests in rotating homogeneous decaying turbulence are shown in Figure 8. These plot the correlation coefficient, ρ_2 , as a function of the filter wave number. The more difficult terms to model are those that have components in the z direction. Thus, only the stress term, τ_{33} , and its divergence, $\partial \tau_{3j} / \partial x_j$, term are shown.

The figures show results for the models presented here (SCDSM (4)-(5) and GCDSM (15)-(17)). Results for two other models are also shown: DS is the original dynamic structure model (8) and SSM is a simple scale similarity model without rescaling by the subgrid kinetic energy.

All models show good results at high wave numbers but are more severely tested at low wave numbers (larger filter sizes). The results show that the rescaling in the DS model gives significantly better results than the SSM model. As the cross correlation terms are added to the DS model to give the SCDSM model, the correlation coefficients improve even more. The GCDSM model also gives good results at larger filter sizes but goes to the wrong limit as the filter size decreases.

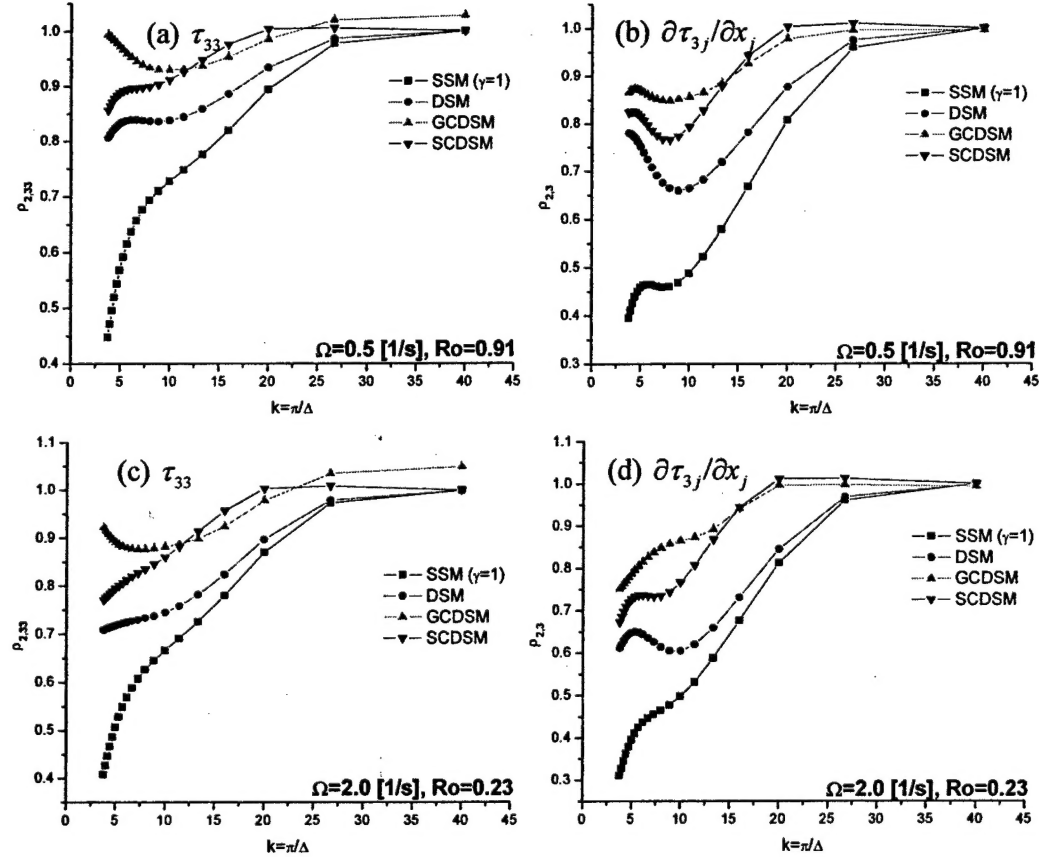


Figure 8: Comparison of the second correlation coefficient, ρ_2 . The filter cutoff wavenumber is defined by $k = \pi/\Delta$: (a) and (b) rotation rate $\Omega = 0.5 [1/s]$ and Rossby number $Ro = 0.91$, (c) and (d) rate $\Omega = 2.0 [1/s]$ and Rossby number $Ro = 0.23$. SSM is a scale similarity model, DSM is the DS model (8), SCDSM is the dynamic structure model with the cross terms (15)-(16) and GCDSM is a gradient model (15)-(17).

Acknowledgment/Disclaimer

This work was sponsored in part by the Air Force Office of Scientific Research, USAF, under grant number F49620-02-1-0348. The views and conclusions contained herein are those of the author and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

References

- Bedford K. W. and Yeo Y. K. (1993), "Conjunctive Filtering Procedures in Surface Water Flow and Transport," in *Large Eddy Simulation of Complex Engineering and Geophysical Flows*, Galperin B. and Orszag S. A., eds., Cambridge University Press, Cambridge, pp. 513—537.
- Chumakov, S. and Rutland, C.J. (2004) "Dynamic Structure Models for Scalar Flux and Dissipation in Large Eddy Simulation," *AIAA Journal*, Vol. 42, No. 6, pp. 1132-1139
- Chumakov, S. and Rutland, C.J. (2005) "Dynamic Structure Subgrid-Scale Models for Large Eddy Simulation," *Int. J. Numerical Methods for Fluids*, to appear.
- Comte-Bellot, G., Corrsin, S. (1966), "The use of a Contraction to Improve the Isotropy of Grid-generated Turbulence," *J. Fluid Mech.*, 25, pp. 657-682
- Cook, A.W. and Riley, J.J. (1994), "A subgrid model for equilibrium chemistry in turbulent flows", *Phys. Fluids* 8, 2248
- Corrsin, S., "Limitations of Gradient Transport Models in Random Walks and in Turbulence," *Adv. Geophys.*, 18 A, pg. 26-60 (1974)
- Dimotakis P.E., (1991), "Turbulent Free Shear Layer Mixing and Combustion," in *High Speed Flight Propulsion Systems*, S.N. Murphy and E.T. Curran, eds., Vol. 137 of *Progress in Astronautics and Aeronautics*, Washington D.C., pp. 265-340
- Eaton J., Johnston J., and Westphal R., "Experimental Study of Flow Reattachment in a Single-sided Sudden Expansion," NASA contractor report 3765, (1986).
- Ferziger J. H., "Higher-level Simulations of Turbulent Flows," in *Computational Methods for Turbulent, Transonic and Viscous Flows*, edited by Essers J. A., Hemisphere Publishing Corporation, (1983).
- Germano M., Piomelli U., Moin P., and Cabot W.H. (1991), "A dynamic subgrid-scale eddy viscosity model", *Phys. Fluids A* 3 (7), 1760-1765
- Ghosal S., Lund T., Moin P., and Aksevoll K. (1995), "A Dynamic Localization Model for Large-Eddy Simulation of Turbulent Flows," *J. Fluid Mech.*, 286, 229-255
- Jimenez, C., Ducros, F., Cuenot, B., and Bedat, B. (2001), "Subgrid scale variance and dissipation of a scalar field in large eddy simulations", *Phys. Fluids* 13 (6), 1748
- Kim W., Menon S. (1995), "A New Dynamic One-Equation Subgrid-Scale Model for Large Eddy Simulation," AIAA 95-0356.
- Kim, W., Menon, S., and Moniga, H.C., (1999), "Large-Eddy Simulation of a Gas Turbine Combustor Flow", *Combust. Sci. and Tech.*, Vol. 143, pp. 25-62
- Kimmel, A.J. and Domaradzki J.A. (2000), "Large eddy simulations of Rayleigh-Bernard convection using subgrid scale estimation model", *Phys. Fluids* 12 (1), 169
- Leonard A. (1974), "Energy Cascade in Large-Eddy Simulations of Turbulent Flows," *Advances in Geophysics A*, 18, pp. 237--248
- Liu S., Meneveau C., Katz J., "On the Properties of Similarity Subgrid-Scale Models as Deduced from Measurements in a Turbulent Jet," *J. Fluid Mech.* 275, 83 (1994).
- Mason, S.D. and Rutland, C.J., 2000 "Turbulence Transport in Spatially Developing Reacting Shear Layers." *Proc. Combust. Inst. 28th International Symposium on Combustion*, Edinburgh Scotland. July 31- Aug. 4, 2000
- Menon S., Yeung P. K., and Kim W. W., Effect of Subgrid Models on the Computed Interscale Energy Transfer in Isotropic Turbulence," *Computer and Fluids*, Vol. 25, No. 2, pp. 165-180. (1996)
- Meneveau, C., and Katz, J., "Scale-Invariance and Turbulence Models for Large-Eddy Simulation," *Annu. Rev. Fluid Mech.* (2000)

- Mohamed, M. S., LaRue, J. C. (1990), "The decay power law in grid-generated turbulence," *J. Fluid Mech.*, Vol. 219, pp. 195-214
- Moin P., "Progress in Large Eddy Simulations of Turbulent Flows," AIAA paper 97-0749, (1997).
- Pierce, C. and Moin, P. (1998), "A dynamic model for subgrid-scale variance and dissipation rate of a conserved scalar", *Phys. Fluids*, vol. 10, No. 12, pp. 3041-3044
- Pomraning E., "Development of Large Eddy Simulation Turbulence Models," Ph.D. Thesis, Dept. of Mechanical Engineering, University of Wisconsin-Madison (2000)
- Pomraning, E. and Rutland, C.J. (2002), "Dynamic One-Equation Nonviscosity Large-Eddy Simulation Model", *AIAA Journal*, Vol. 40, No. 4, pp. 689-701
- Pope, S. (2000), *Turbulent Flows*, Cambridge Univ. Press.
- Shimomura, Yutaka (1999), "A family of dynamic subgrid-scale models consistent with asymptotic material frame indifference," *J. of the Physical Society of Japan*, 68(8):2483-2486.
- Speziale, Charles G. (1985), "Subgrid scale stress models for the large-eddy simulation of rotating turbulent flows," *Geophys. Astrophys. Fluid Dynamics*, 33:199-222.
- Speziale C.G., Erlebacher G., Zang T.A., and Hussaini M.Y. (1988), "The subgrid-scale modeling for compressible turbulence", *Phys. Fluids* 31 (4), 9406.

Publications:

- Chumakov, S. and Rutland, C.J. (2004) "Dynamic Structure Models for Scalar Flux and Dissipation in Large Eddy Simulation," *AIAA Journal*, Vol. 42, No. 6, pp. 1132-1139
- Chumakov, S. and Rutland, C.J. (2005) "Dynamic Structure Subgrid-Scale Models for Large Eddy Simulation," *Int. J. Numerical Methods for Fluids*, to appear.

Personnel Supported

Sergei Chumakov	Graduate Student, University of Wisconsin-Madison
Robert Gladney	Graduate Student, University of Wisconsin-Madison
Hao Lu	Graduate Student, University of Wisconsin-Madison
Christopher J. Rutland	Professor, University of Wisconsin-Madison